William D. Gropp

Senior Computer Scientist
Mathematics and Computer Science Division
Argonne National Laboratory
Argonne, IL 60439

Education:

Stanford University, Stanford, CA
  Ph.D. in Computer Science (January 1982)
  M.S. in Computer Science (June 1980)

University of Washington, Seattle, WA
  M.S. in Physics (June 1978)

Case Western Reserve University, Cleveland, OH
  B.S. in Mathematics (May 1977)

Professional Experience:

Argonne National Laboratory
  Senior Computer Scientist
  March 1996 to present

  Computer Scientist
  March 1990 to March 1996

  Fellow of the Argonne Accelerator Institute
  February 2007 to present

  Associate Division Director
  March 2000 to March 2006

  Deputy Scientific Director of the High-Performance Computing Research Facility
  September 1990 to April 1997

University of Chicago
  Senior Scientist, Computer Science Department
  2000 to present (joint appointment with Argonne)

  Senior Fellow, Computation Institute of Argonne National Laboratory
  and the University of Chicago
  1999 to present

Yale University
  Associate Professor of Computer Science
  July 1988 to February 1990

  Assistant Professor of Computer Science
  January 1982 to July 1988

Awards, Honors, and Patents:

ACM Fellow
U.S. Patent 7076553, awarded July 11, 2006.
Euro PVMMPI 2006 Best Papers (2)
R&D100 for MPICH2 in 2005
SC2003 Best Poster Award, with Suren Byna, Rajeev Thakur, and Xian-He Sun
Beale-Orchard-Hays Honorable Mention, 2000, with Jorge Moré
Gordon Bell Prize, 1999, with Anderson, Kaushik, Keyes, and Smith

Recent Professional Activities:

Conference Organizing Committee Chair:
> SIAM Parallel Processing 2006 (joint with Charbel Farhat)

Conference Technical Program Chair:
> IEEE Cluster 2002, IEEE Cluster 2006, WoCo9 2006.

Conference Technical Program Papers Chair:
> SC2006 (joint with Daniel Reed)

Conference Committees (since 2002):
> IEEE Cluster 2003, 2004
> ACM/IEEE Supercomputing 2002, 2003, 2004, 2005
> EuroPVMMPI 2002, 2003, 2004, 2005, 2006, 2007
> ISHPC02, WIMPS02, IWIA03, ICPP-2003, IPDPS 2004, SIAM PP04, SciDAC 2005,
> Frontiers of Extreme Computing 2005, CESC2006, IWIA07, ParCo 2007, HPCC07, MHSN2007,
> IPDPS08

Series editor:
> MIT Press Scientific and Engineering Computation

Editorial boards:
> Concurrency and Computation
> International Journal of High Performance Computing Applications
> International Journal of Computational Science and Engineering

Scientific Advisory Board, Aachen Institute for Advanced Study in Computational Engineering
Science (AICES) (2007-current)

Gordon Bell Prize Committee:
> Member (2002,2006), Chair (2003,2004,2005)

IEEE Computer Society Seymour Cray Award Committee (2004)
IFIP Working Group 2.5 (Numerical Software), 2003-present
Membership in professional societies:
> SIAM, ACM, IEEE

Chair, SIAM Activity group on Supercomputing 2003–2006

Teaching and Mentoring

Ph.D. Dissertation Committees:
John Ellis, Yale University, Department of Computer Science, 1985
Kai Li, Yale University, Department of Computer Science, 1986
Ye-Yang Sun, Yale University, Department of Engineering and Applied Science, 1987
Leslie Greengard, Yale University, Department of Computer Science, 1987

Elizabeth Jessup, Yale University, Department of Computer Science, 1989
Zhijing George Mou, Yale University, Department of Computer Science, 1990
Ali Ecder, Yale University, Department of Enginnering and Applied Science, 1992
Nickolas S. Jovanovic, Yale University, Department of Engineering and Applied Science, 1997
Dinesh Kaushik, Old Dominion University, 2002
Jeffrey Evans, Illinois Institute of Technology, 2005
Pierre Lemantier, Universite Paris Sud, 2006

Post Doctoral Students Supervised:
David Keyes, Yale University
Barry Smith (Wilkinson Fellow), Argonne National Laboratory
Lois Curfman McInnes, Argonne National Laboratory
Rajeev Thakur, Argonne National Laboratory
Dinesh Kaushik, Argonne National Laboratory
Robert Ross, Argonne National Laboratory
Darius Buntinas, Argonne National Laboratory
Pavan Balaji, Argonne National Laboratory

Summer Students Supervised:
Erin Martin, Carrie Wilson, Thomas VanDrunen, Alison Baker, Jason Karlin, Suren Byna, Ernie Chan.

Classes Taught at Yale Included:
Ordinary Differential Equations
Introduction to Applied Computation (Programming with FORTRAN)
Fortran for Scientists and Engineers
Computer Graphics
Time Dependent Partial Differential Equations
Scientific Computing with SIMD Parallel Computers
Reading Course in Numerical Analysis

Selected Tutorials Taught:

1. E. Lusk, W. Gropp, R. Ross, and R. Thakur, "Advanced MPI: I/O and One-Sided Communication," SC2006, Tampa, FL, November 2006.

2. W. Gropp and R. Thakur, "MPI on the Grid," CCGrid 2006, Singapore, May, 2006.

3. E. Lusk, W. Gropp, R. Ross, and R. Thakur, "Advanced MPI: I/O and One-Sided Communication," SC2005, Seattle, WA, November 2005.

4. W. Gropp and E. Lusk, "Using MPI-2: A Problem-Based Approach," PVMMPI 2005, Sorrento, Italy, 2005.

5. B. Smith, M. Knepley, D. Kaushik, W. Gropp, "Introduction to PETSc," DD16, New York, NY, January, 2005.

6. W. Gropp, E. Lusk, R. Ross, and R. Thakur, "Advanced MPI: I/O and One-Sided Communication," SC2004, Pittsburgh, PA, November, 2004.

7. W. Gropp, E. Lusk, "Using MPI-2: A Problem-Based Approach," PVMMPI 2004, Budapest, Hungary, September, 2004.

8. W. Gropp, E. Lusk, R. Ross, and R. Thakur, "Using MPI-2: A Tutorial on Advanced Features of the Message-Passing Interface Standard," SC2003, Phoenix, AZ, November, 2003.

9. W. Gropp, "Parallel Programming with MPI," Cluster School, Merida, Venezula, October, 2003.

10. W. Gropp and E. Lusk, "High-Level Programming in MPI," PVMMPI 2003, Venice, Italy, September, 2003.

11. W. Gropp, "PETSc," ACTS Workshop 2003, Berkeley, CA, August, 2003.

12. W. Gropp, D. Keyes, "Introduction to Domain Decomposition with PETSc," Domain Decomposition 15, Berlin, Germany, July, 2003.

13. W. Gropp, E. Lusk, R. Ross, and R. Thakur, "Using MPI-2: A Tutorial on Advanced Features of the Message-Passing Interface Standard," SC2002, Baltimore, MD, November, 2002.

14. W. Gropp, D. Keyes, "PETSc Tutorial," Peking University, Beijing, China, July 2002.

15. W. Gropp, E. Lusk, R. Ross, and R. Thakur, "Using MPI-2: A Tutorial on Advanced Features of the Message-Passing Interface Standard," SC2001, Denver, CO, November, 2001.

16. W. Gropp, "Advanced Cluster Programming with MPI," Cluster 2001, Newport Beach, CA, October, 2001.

17. W. Gropp, E. Lusk, R. Thakur, "Using MPI-2: A Tutorial on Advanced Features of the Message-Passing Interface," SC2000, Dallas, TX, November, 2000.

18. S. Balay, K. Buschelman, W. Gropp, L. Curfman McInnes, and B. Smith, "PETSc Tutorial: Numerical Software Libraries for the Scalable Solution of PDEs," Workshop on the ACTS Toolkit, Berkeley, CA, September, 2000.

19. S Balay, W. Gropp, L. Curfman McInnes, B. Smith, "Tutorial on the Portable, Extensible Toolkit for Scientific computation (PETSc)," DD13, Lyon, France, October, 2000.

20. W. Gropp, "High Performance MPI," CASC, Lawrence Livermore National Laboratory, May, 2000.

21. W. Gropp, "Short Course on the Portable, Extensible Toolkit for Scientific computation (PETSc),"4th Annual National Symposium on Computational Science and Engineering (ANSCSE4), Bangkok, Thailand, March, 2000.

22. W. Gropp, E. Lusk, R. Thakur, "Tuning MPI Applications for Peak Performance," SC99, Portland, OR, November, 1999.

23. W. Gropp, MPI Portion of "How to Run A Beowulf Cluster," (Thomas Sterling organizer), SC99, Portland, OR, November, 1999.

24. W. Gropp, E. Lusk, R. Thakur, "Using MPI-1 and MPI-2," PVMMPI'99, Barcelona, Spain, September, 1999.

25. W. Gropp, "Introduction to the Message Passing Interface," Summer Institute for Advanced Computation, Wright State University, August, 1999.

26. S. Balay, W. Gropp, L. Curfman McInnes, "PETSc Tutorial", Parallel CFD'99, Williamsburg, VA, May, 1999.

27. W. Gropp, "Intermediate MPI," NRL, Monterey, CA, April, 1999.

28. W. Gropp, "PETSc Tutorial," SIAM Parallel Processing, San Antonio, TX, March 1999.

29. W. Gropp, "Introduction to MPI," as part of "High Performance Programming," Technical University of Denmark, Lyngby, Denmark, December 1998.

30. W. Gropp, E. Lusk, R. Thakur, "Tuning MPI Applications for Peak Performance," SC98, Orlando, FL, November, 1998.

31. W. Gropp, "Portable High Performance Parallel I/O and MPI," Utrecht, The Netherlands, February, 1998.

32. W. Gropp, E. Lusk, and R. Thakur, "Introduction to Performance Issues in Using MPI for Communication and I/O,", HPDC-7, Chicago, IL, July, 1998.

33. W. Gropp, "PETSc Tutorial," SC97, November, 1997.

1   Books

[1] William Gropp, Ewing Lusk, and Anthony Skjellum. *Using MPI: Portable Parallel Programming with the Message-Passing Interface.* MIT Press, Cambridge, MA, 1994.

[2] B. F. Smith, P. E. Bjørstad, and W. D. Gropp. *Domain Decomposition: Parallel Multilevel Methods for Elliptic Partial Differential Equations.* Cambridge University Press, New York, 1996.

[3] William Gropp, Steven Huss-Lederman, Andrew Lumsdaine, Ewing Lusk, Bill Nitzberg, William Saphir, and Marc Snir. *MPI - The Complete Reference: Volume 2, The MPI-2 Extensions.* MIT Press, Cambridge, MA, USA, 1998.

[4] William Gropp, Ewing Lusk, and Anthony Skjellum. *Using MPI: Portable Parallel Programming with the Message Passing Interface,* 2nd edition. MIT Press, Cambridge, MA, 1999.

[5] William Gropp, Ewing Lusk, and Rajeev Thakur. *Using MPI-2: Advanced Features of the Message-Passing Interface.* MIT Press, Cambridge, MA, 1999.

[6] Jack Dongarra, Ian Foster, Geoffrey Fox, William Gropp, Ken Kennedy, Linda Torczon, and Andy White, editors. *Sourcebook of Parallel Computing.* Morgan Kaufmann, 2003.

[7] William Gropp, Ewing Lusk, and Thomas Sterling, editors. *Beowulf Cluster Computing with Linux.* MIT Press, 2nd edition, 2003.

2 Book Chapters

[1] William Gropp. *Sourcebook of Parallel Computing*, chapter Parallel Computer Architectures, pages 15–42. Morgan Kaufmann, 2003.

[2] Ian Foster, William Gropp, and Carl Kesselman. *Sourcebook of Parallel Computing*, chapter Message Passing and Threads, pages 313–329. Morgan Kaufmann, 2003.

[3] Rajeev Thakur and William Gropp. *Sourcebook of Parallel Computing*, chapter Parallel I/O, pages 331–355. Morgan Kaufmann, 2003.

[4] William Gropp. *Sourcebook of Parallel Computing*, chapter The 2-D Poisson Problem, pages 469–480. Morgan Kaufmann, 2003.

[5] Satish Balay, William Gropp, Lois Curfman McInnes, and Barry F. Smith. *Sourcebook of Parallel Computing*, chapter Software for the Scalable Solution of Partial Differential Equations, pages 621–647. Morgan Kaufmann, 2003.

[6] William Gropp. *Beowulf Cluster Computing with Linux*, chapter So You Want to Use a Cluster, pages 1–17. MIT Press, 2003.

[7] Ewing Lusk, William Gropp, and Ralph Butler. *Beowulf Cluster Computing with Linux*, chapter An Introduction to Writing Parallel Programs, pages 171–206. MIT Press, 2003.

[8] William Gropp and Ewing Lusk. *Beowulf Cluster Computing with Linux*, chapter Parallel Programming with MPI, pages 207–243. MIT Press, 2003.

[9] William Gropp and Ewing Lusk. *Beowulf Cluster Computing with Linux*, chapter Advanced Topics in MPI Programming, pages 245–278. MIT Press, 2003.

[10] Rajeev Thakur, William Gropp, and Ewing Lusk. *Scalable Input/Output*, chapter ADIO: A Framework for High-Performance, Portable Parallel I/O, pages 111–134. MIT Press, 2004.

[11] William D. Gropp. *Accuracy and Reliability in Scientific Computing*, chapter Issues in Accurate and Reliable Use of Parallel Computing in Numerical Programs. SIAM, 2005.

[12] Ricky A. Kendall, Masha Sosonkina, William D. Gropp, Robert W. Numrich, and Thomas Sterling. *Numerical Solution of Partial Differential Equations on Parallel Computers*, chapter Parallel Programming Models Applicable to Cluster Computing and Beyond, pages 3–54. Number 51 in Lecture Notes in Computational Science and Engineering. Springer, 2006.

[13] William D. Gropp and Andrew Lumsdaine. *Parallel Processing for Scientific Computing*, chapter Parallel Tools and Environments: A Survey, pages 223–232. SIAM, 2006.

[14] Boyana Norris, Albert Hartono, and William Gropp. *Petascale Computing: Algorithms and Applications*, chapter Annotations for Productivity and Performance Portability. Computational Science. Chapman & Hall / CRC Press, Taylor and Francis Group, 2007. Preprint ANL/MCS-P1392-0107.

3 Workshop and Meeting Reports

[1] David Keyes, Philip Colella, Thom H. Dunning, and William D. Gropp. A science-based case for large-scale simulation, volume 1, July 2003. Office of Science, U.S. Department of Energy.

[2] Hans P. Zima, editor. Workshop on high-productivity programming languages and models, 2004. Report of the workshop.

[3] Jennifer M. Schopf, editor. Grid performance workshop 2004 report, 2004.

[4] International workshop on advanced computational materials science: Application to fusion and generation-IV fission reactors, 2004. Also ORNL/TM-2004/132.

[5] David Keyes, Philip Colella, Thom H. Dunning, and William D. Gropp. A science-based case for large-scale simulation, volume 2, September 2004. Office of Science, U.S. Department of Energy.

4 Journal Articles

[1] William D. Gropp. A test of moving mesh refinement for 2-D scalar hyperbolic problems. *SIAM Journal on Scientific and Statistical Computing*, 1(2):191–197, June 1980.

[2] William D. Gropp. Solving PDEs on loosely-coupled parallel processors. *Parallel Computing*, 5(1-2):165–173, July 1987. Proceedings of the international conference on vector and parallel computing—issues in applied research and development (Loen, 1986).

[3] David E. Keyes and William D. Gropp. A comparison of domain decomposition techniques for elliptic partial differential equations and their parallel implementation. *SIAM Journal on Scientific and Statistical Computing*, 8(2):S166–S202, March 1987. Reprinted in Selected Papers from the Second Conference on Parallel Processing for Scientific Computing (C. W. Gear & R. G. Voigt, eds., SIAM, 1987).

[4] William D. Gropp. Local uniform mesh refinement with moving grids. *SIAM Journal on Scientific and Statistical Computing*, 8(3):292–304, May 1987.

[5] W. Gropp. Local uniform mesh refinement on loosely-coupled parallel processors. *I. J. Comp. Math. Appl.*, 15:375–389, 1988.

[6] William D. Gropp and David E. Keyes. Complexity of parallel implementation of domain decomposition techniques for elliptic partial differential equations. *SIAM Journal on Scientific and Statistical Computing*, 9(2):312–326, March 1988.

[7] William D. Gropp and I. C. F. Ipsen. Recursive mesh refinement on hypercubes. *Nordisk Tidskr. Informationsbehandling (BIT)*, 29:186–211, 1989.

[8] William D. Gropp and David E. Keyes. Domain decomposition on parallel computers. *Impact Comput. Sci. Eng.*, 1:421–439, 1989.

[9] David E. Keyes and William D. Gropp. Domain decomposition techniques for the parallel solution of nonsymmetric systems of elliptic boundary value problems. *Applied Numerical Mathematics: Transactions of IMACS*, 6(4):281–301, May 1990.

[10] H. Berryman, J. Saltz, W. Gropp, and R. Mirchandaney. Krylov methods preconditioned with incompletely factored matrices on the CM-2. *Journal of Parallel and Distributed Computing*, 8(2):186–190, February 1990.

[11] Leslie Greengard and William D. Gropp. A parallel version of the fast multipole method. *Computers and Mathematics with Applications*, 20:63–71, 1990.

[12] William D. Gropp and Edward Smith. Computational fluid dynamics on parallel processors. *Computers and Fluids*, 18:289–304, 1990.

[13] Xiao-Chuan Cai, William D. Gropp, and David E. Keyes. Convergence rate estimate for a domain decomposition method. *Numerische Mathematik*, 61(2):153–169, 1992.

[14] W. D. Gropp and D. E. Keyes. Domain decomposition with local mesh refinement. *SIAM J. Sci. Stat. Comput.*, 13:967–993, 1992.

[15] W. D. Gropp and D. E. Keyes. Parallel performance of domain-decomposed preconditioned Krylov methods for PDEs with locally uniform refinement. *SIAM Journal on Scientific and Statistical Computing*, 13:128–145, 1992.

[16] W. D. Gropp and D. E. Keyes. Domain decomposition methods in computational fluid dynamics. *Int. J. Numer. Meth. Fluids*, 14:147–165, 1992.

[17] I. Foster, W. Gropp, and R. Stevens. The parallel scalability of the spectral transform method. *Monthly Weather Review*, 120(5):835–850, 1992.

[18] Xiao-Chuan Cai, William D. Gropp, and David E. Keyes. A comparison of some domain decomposition and *ILU* preconditioned iterative methods for nonsymmetric elliptic problems. *Numerical linear algebra with applications*, 1(5):477–504, 1994.

[19] Message Passing Interface Forum. MPI: A message passing interface standard. *International Journal of Supercomputer Applications*, 8(3/4):159–416, 1994.

[20] K. Forsman, W. Gropp, L. Kettunen, D. Levine, and J. Salonen. Solution of dense systems of linear equations arising from integral equation formulations. *IEEE Antennas and Propagation Magazine*, pages 96–100, December 1995.

[21] W. D. Gropp and E. Lusk. Experiences with the IBM SP1. *IBM Systems Journal*, 34(2):249–262, 1995.

[22] Anthony Skjellum, Ewing Lusk, and William Gropp. Early applications in the Message-Passing Interface (MPI). *International Journal of Supercomputer Applications and High Performance Computing*, 9(2):79–94, Summer 1995.

[23] William D. Gropp, Hans Kaper, G. Leaf, D. Levine, V. Vinokur, and M. Palumbo. Numerical simulation of vortex dynamics in high-t_c superconductors. *J. Comp. Physics*, 123:254–266, 1996.

[24] W. Gropp, E. Lusk, N. Doss, and A. Skjellum. A high-performance, portable implementation of the MPI message passing interface standard. *Parallel Computing*, 22(6):789–828, September 1996.

[25] R. Thakur, W. Gropp, and E. Lusk. An experimental evaluation of the parallel I/O systems of the IBM SP and Intel Paragon using a production application. *Lecture Notes in Computer Science*, 1127, 1996.

[26] Barry Smith and William Gropp. The design of data-structure-neutral libraries for the iterative solution of sparse linear systems. *Scientific Programming*, 5:329–336, 1996.

[27] W. Gropp and E. Lusk. A high-performance MPI implementation on a shared-memory vector supercomputer. *Parallel Computing*, 22(11):1513–1526, January 1997.

[28] W. Gropp and E. Lusk. Sowing MPICH: A case study in the dissemination of a portable environment for parallel scientific computing. *The International Journal of Supercomputer Applications and High Performance Computing*, 11(2):103–114, Summer 1997.

[29] Message Passing Interface Forum. MPI2: A message passing interface standard. *High Performance Computing Applications*, 12(1–2):1–299, 1998.

[30] Rajeev Thakur, Ewing Lusk, and William Gropp. I/O in parallel applications: The weakest link. *The International Journal of High Performance Computer Applications*, 12(4, part 2):389–395, 1998.

[31] X-C Cai, William D. Gropp, David E. Keyes, R. G. Melvin, and D. P. Young. Parallel Newton-Krylov-Schwarz algorithms for the transonic full potential equation. *SIAM Journal of Scientific Computing*, 19:246–265, January 1998. Also ICASE report TR 96-39.

[32] William Gropp and Ewing Lusk. PVM and MPI are completely different. *Future Generation Computer Systems*, 1999. Submitted as part of a PVMMPI special issue.

[33] I. Foster, J. Geisler, W. Gropp, N. Karonis, E. Lusk, G. Thiruvathukal, and S. Tuecke. A wide-area implementation of the Message Passing Interface. *Parallel Computing*, 24(12–13):1735–1749, November 1998.

[34] David Levine, William Gropp, Kimmo Forsman, and Lauri Kettunen. Parallel computation of three-dimensional nonlinear magnetostatic problems. *Concurrency Practice and Experience*, 11(2):109–120, February 1999.

[35] Omer Zaki, Ewing Lusk, William Gropp, and Deborah Swider. Toward scalable performance visualization with Jumpshot. *High Performance Computing Applications*, 13(2):277–288, Fall 1999.

[36] William Gropp, David E. Keyes, Lois C. McInnes, and M. D. Tidriri. Globalized Newton-Krylov-Schwarz algorithms and software for parallel implicit CFD. *High Performance Computing Applications*, 14(2):102–136, 2000.

[37] W. D. Gropp, D. K. Kaushik, D. E. Keyes, and B. F. Smith. High-performance parallel implicit CFD. *Parallel Computing*, 27:337–362, 2001.

[38] Ralph Butler, William Gropp, and Ewing Lusk. Components and interfaces of a process management system for parallel programs. *Parallel Computing*, 27(11):1417–1429, October 2001.

[39] W. D. Gropp, D. K. Kaushik, D. E. Keyes, and B. F. Smith. High performance parallel implicit CFD. *Parallel Computing*, 27(4):337–362, 2001.

[40] Rajeev Thakur, William Gropp, and Ewing Lusk. Optimizing noncontiguous accesses in MPI-IO. *Parallel Computing*, 28(1):83–105, January 2002.

[41] Mark Baker, Daniel Katz, William Gropp, and Thomas Sterling. Special issue: Cluster 2001. *Concurrency and Computation: Practice and Experience*, 15(7–8):623–624, 2003.

[42] William D. Gropp and Ewing Lusk. Fault tolerance in MPI programs. *International Journal of High Performance Computer Applications*, 18(3):363–372, 2004.

[43] Rajeev Thakur, Rolf Rabenseifner, and William Gropp. Optimization of collective communication operations in MPICH. *International Journal of High Performance Computer Applications*, 19(1):49–66, 2005.

[44] George Almási, Charles Archer, Jose G. Casta nos, J. A. Gunnels, C. Chris Erway, Philip Heidelberger, Xavier Martorell, Jose E. Moreira, Kurt Pinnow, Joe Ratterman, Burkhard Steinmacher-Burow, William Gropp, and Brian Toonen. Design and implementation of message-passing services for the Blue Gene/L supercomputer. *IBM Journal of Research and Development*, 49(2/3):393–406, March/May 2005. Available at `http://www.research.ibm.com/journal/rd49-23.html`.

[45] Rajeev Thakur, William Gropp, and Brian Toonen. Optimizing the synchronization operations in MPI one-sided communication. *High Performance Computing Applications*, 19(2):119–128, 2005.

[46] Christopher Falzone, Anthony Chan, Ewing Lusk, and William Gropp. A portable method for finding user errors in the usage of mpi collective operations. *International Journal of High Performance Computing Applications*, 21(2):155–165, 2007.

[47] Baifei Shen, Yuelin Li, Karoly Nemeth, Hairong Shang, Yong chul Chae, Robert Soliday, Robert Crowell, Edward Frank, William Gropp, and John Cary. Electron injection by a nanowire in the bubble regime. *Physics of Plasmas*, 14, 2007.

5   Proceedings

[1] William Gropp. Parallel programming tools for distributed memory computers. In Adrian Tentner, editor, *High Performance Computing: Grand Challenges in Computer Simulation*, pages 166–169. The Society for Computer Simulation, 1993.

[2] D. L. Boley, William D. Gropp, and M. M. Theimer. A method for constructing preprocessors. In *Conference on the Computing Environment for Mathematical Software*. JPL and ACM-SIGNUM, July 1981. JPL Publication 81-67.

[3] W. D. Gropp. Numerical linerar algebra on workstations. In *Proc. Army Research Office Workshop on Microcomputers in Scientific Computing*, 1985.

[4] William D. Gropp. A system for numerical linear algebra. In A. Wouk, editor, *New Computing Environments: Microcomputers in Large-Scale Computing*, pages 26–38, Philadelphia, 1987. SIAM.

[5] William D. Gropp. Local uniform mesh refinement on parallel processors. In P. Deuflhard and B. Enquist, editors, *Large Scale Scientific Computing*, Boston, 1987. Birkhäuser.

[6] William D. Gropp. Adaptive methods for hyperbolic problems on local memory parallel processors. In M. H. Schultz, editor, *Numerical Algorithms for Modern Computer Architectures*, pages 77–84, New York, 1988. Springer-Verlag.

[7] William Gropp and Edward Smith. Computational fluid dynamics on parallel processors. In *1st National Fluid Dynamics Congress, Part 1*, pages 612–619. AIAA/ASME/SIAM/APS, American Institute of Aeronautics and Astronautics, July 1988.

[8] William D. Gropp and Martin Schultz. A highly parallel method for an underwater acoustics problem. In *Proceedings of the Fourth International Conference on Supercomputing, Santa Clara, California*, 1989.

[9] H. S. Barryman, William D. Gropp, and J. Saltz. Krylov methods and the CM/2. In *Proceedings of the Fourth International Conference on Supercomputing, Santa Clara, California*, 1989.

[10] William D. Gropp and David Foulser. CLAM: A programming language for interactive supercomputing and visualization. In *Proceedings of the Fourth International Conference on Supercomputing, Santa Clara, California*, 1989.

[11] William D. Gropp. Dynamic grid manipulation for PDEs on hypercube parallel processors. In A. Wouk, editor, *Parallel Processing and Medium-Scale Multiprocessors*, pages 192–203, Philadelphia, 1989. SIAM.

[12] Leslie Greengard and William D. Gropp. A parallel version of the fast multipole method. In Gary Rodrigue, editor, *Proceedings of the 3rd Conference on Parallel Processing for Scientific Computing*, pages 213–222, Philadelphia, PA, USA, December 1989. SIAM Publishers.

[13] W. D. Gropp and I. C. F. Ipsen. A Gray code scheme for local uniform mesh refinement on hypercubes. In Garry Rodrigue, editor, *Parallel Processing for Scientific Computing: Proceedings of the Third SIAM Conference on Parallel Processing for Scientific Computing, Los Angeles, California, December 1–4, 1987*, pages 202–206, Philadelphia, 1987. SIAM Publ.

[14] William D. Gropp and David E. Keyes. Parallel domain decomposition with local mesh refinement. In Danny C. Sorensen, Jack Dongarra, Paul Messina, and Robert G. Voigt, editors, *Proceedings of the 4th Conference on Parallel Processing for Scientific Computing*, pages 295–296, Philadelphia, PA, USA, December 1989. SIAM Publishers.

[15] W. D. Gropp and D. E. Keyes. Domain decomposition on parallel computers. In T. F. Chan, R. Glowinski, J. Périaux, and O. B. Widlund, editors, *Domain Decomposition Methods*, pages 260–288. SIAM, Philadelphia, 1989.

[16] D. E. Keyes, W. D. Gropp, and A. Ecder. Domain decomposition techniques for large sparse nonsymmetric systems arising from elliptic problems with first–order terms. In J. H. Kane and A. D. Carlson, editors, *Proceedings of a Symposium on the Solution of Super Large Problems in Computational Mechanics*, New York, 1989. Plenum.

[17] D. E. Keyes and W. D. Gropp. Domain decomposition techniques for nonsymmetric systems of equations: examples from computational fluid dynamics. In T. F. Chan, R. Glowinski, J. Périaux, and O. B. Widlund, editors, *Domain Decomposition Methods*, pages 321–339. SIAM, Philadelphia, 1989.

[18] Z. George Mou, David E. Keyes, and William D. Gropp. Balanced divide-and-conquer algorithms for the fine-grained parallel direct solution of dense and banded triangular linear systems and their connection machine implementation. In Danny C. Sorensen, Jack Dongarra, Paul Messina, and Robert G. Voigt, editors, *Proceedings of the 4th Conference on Parallel Processing for Scientific Computing*, pages 386–387, Philadelphia, PA, USA, December 1989. SIAM Publishers.

[19] D. E. Foulser and W. D. Gropp. CLAM and CLAMShell: An interactive front-end for parallel computing and visualization. In Pen-Chung Yew, editor, *Proceedings of the 1990 International Conference on Parallel Processing. Volume 3: Algorithms and Architectures*, pages 35–43, Urbana-Champaign, IL, August 1990. Pennsylvania State University Press.

[20] W. D. Gropp and D. E. Keyes. A domain decomposition method with locally uniform mesh refinement. In T. F. Chan, R. Glowinski, J. Périaux, and O. B. Widlund, editors, *Third International Symposium on Domain Decomposition Methods for Partial Differential Equations*, pages 115–129, Philadelphia, 1990. SIAM.

[21] William D. Gropp and Martin H. Schultz. High performance parabolic equation solvers. In D. Lee, A. Cakmak, and R. Vichnevetsky, editors, *Computational Acoustics*, volume 1. Elsevier Science Pub., 1990.

[22] William Gropp. Parallel computing and the solution of partial differential equations (abstract). In Irene O. Macke, editor, *Transactions of the American Nuclear Society*, volume 62, page 269. American Nuclear Society, November 1990. Invited Paper.

[23] William Gropp. Visual artifacts in boundary conditions. In A. Louise Perkins and Jeffrey S. Scroggs, editors, *Proceedings for the ICASE Workshop on Heterogeneous Boundary Conditions*, number NASA Contractor Report 187630, pages 1–3. ICASE, August 1991.

[24] Tony F. Chan, William Gropp, and David E. Keyes. Domain decomposed preconditionings for transport operators. In A. Louise Perkins and Jeffrey S. Scroggs, editors, *Proceedings for the ICASE Workshop on Heterogeneous Boundary Conditions*, number NASA Contractor Report 187630, pages 12–30. ICASE, August 1991.

[25] I. Foster, W. Gropp, and R. Stevens. Parallel scalability of the spectral transform method. In Jack Dongarra, Ken Kennedy, Paul Messina, Danny C. Sorensen, and Robert G. Voigt, editors, *Proceedings of the 5th SIAM Conference on Parallel Processing for Scientific Computing*, pages 307–314, Houston, TX, March 1991. SIAM.

[26] W. D. Gropp and D. E. Keyes. Parallel domain decomposition and the solution of nonlinear systems of equations. In R. Glowinski, Yu. A. Kuznetsov, G. A. Meurant, J. Périaux, and O. B. Widlund, editors, *Fourth International Symposium on Domain Decomposition Methods for Partial Differential Equations*, pages 373–381, Philadelphia, 1991. SIAM.

[27] D. E. Keyes and W. D. Gropp. Domain-decomposable preconditioners for second–order upwind discretizations of multicomponent systems. In R. Glowinski, Yu. A. Kuznetsov, G. A. Meurant, J. Périaux, and O. B. Widlund, editors, *Fourth International Symposium on Domain Decomposition Methods for Partial Differential Equations*, pages 129–139, Philadelphia, 1991. SIAM.

[28] Xiao-Chuan Cai, William D. Gropp, and David E. Keyes. A comparison of some domain decomposition algorithms for nonsymmetric elliptic problems. In Tony F. Chan, David E. Keyes, Gérard A. Meurant, Jeffrey S. Scroggs, and Robert G. Voigt, editors, *Fifth International Symposium on Domain Decomposition Methods for Partial Differential Equations*, Philadelphia, PA, USA, 1992. SIAM.

[29] William D. Gropp and David E. Keyes. Domain decomposition as a mechanism for using asymptotic methods. In H. G. Kaper and M. Garbey, editors, *Asymptotic and Numerical Methods for Partial Differential Equations with Critical Parameters*, pages 93–106. Kluwer, Dordrecht, 1992.

[30] William D. Gropp. Parallel computing and domain decomposition. In Tony F. Chan, David E. Keyes, Gérard A. Meurant, Jeffrey S. Scroggs, and Robert G. Voigt, editors, *Fifth International Symposium on Domain Decomposition Methods for Partial Differential Equations*, Philadelphia, PA, USA, 1992. SIAM.

[31] William D. Gropp and David E. Keyes. Semi-structured refinement and parallel domain decomposition methods. In P. Mehrotra et al., editor, *Unstructured Scientific Computation on Multiprocessors*, pages 187–203. MIT Press, 1992.

[32] Ralph Butler, William D. Gropp, and Ewing Lusk. Developing applications for a heterogeneous computing environment. In *Proc. Workshop on Heterogeneous Processing*, pages 77–83, Los Alamitos, California, 1993. IEEE.

[33] William Gropp. Parallel programming tools for distributed-memory computers. In *Proc. of the 1993 SCS Simulation Multiconference*, March 1993.

[34] N. Galbreath, W. Gropp, D. Gunter, D. Leaf, and D. Levine. Parallel solution of the three-dimensional, time-dependent Ginzburg-Landau equation. In Linda R. Petzold, Richard F. Sincovec, David E. Keyes, Michael R. Leuze, and Daniel A. Reed, editors, *Proceedings of the 6th SIAM Conference on Parallel Processing for Scientific Computing*, pages 160–164, Norfolk, VI, March 1993. SIAM Press.

[35] N. Galbreath, W. Gropp, and D. Levine. Applications-driven parallel I/O. In *Proceedings of Supercomputing '93*, pages 462–471. IEEE Computer Society Press, 1993. Reprinted in the book "High Performance Storage and Parallel I/O" (`http://www.buyya.com/superstorage/`, 2001, pages 539–547).

[36] L. Kettunen, K. Forsman, D. Levine, and W. Gropp. Solutions of team problem #13 using integral equations in a sequential and parallel computing environment. In *Proceedings of the Miami TEAM Workshop*. Florida International University, Department of Electrical Engineering and Computing Science, December 1993.

[37] X.-C. Cai, W. D. Gropp, D. E. Keyes, and M. D. Tidriri. Parallel implicit methods for aerodynamics. In *Domain Decomposition Methods in Scientific and Engineering Computing: Proceedings of the Seventh International Conference on Domain Decomposition*, volume 180 of *Contemporary Mathematics*, pages 465–470, Providence, Rhode Island, 1994. American Mathematical Society.

[38] X.-C. Cai, William D. Gropp, David E. Keyes, and M. D. Tidriri. Newton-Krylov-Schwarz methods in CFD. In F. Hebeker and R. Rannacher, editors, *Proceedings of the International*

Workshop on Numerical Methods for the Navier-Stokes Equations, Notes in Numerical Fluid Mechanics, pages 17–30, Braunschweig, 1994. Vieweg Verlag.

[39] W. D. Gropp, D. E. Keyes, and J. S. Mounts. Implicit domain decomposition algorithms for steady, compressible aerodynamics. In *Domain Decomposition Methods in Science and Engineering: The Sixth International Conference on Domain Decomposition*, volume 157 of *Contemporary Mathematics*, pages 203–213, Providence, Rhode Island, 1994. American Mathematical Society.

[40] W. Gropp and B. Smith. Scalable, extensible, and portable numerical libraries. In *Proceedings of the Scalable Parallel Libraries Conference, October 6–8, 1993, Mississippi State, Mississippi*, pages 87–93, 1109 Spring Street, Suite 300, Silver Spring, MD 20910, USA, 1994. IEEE Computer Society Press.

[41] W. Gropp and E. Lusk. The MPI communication library: its design and a portable implementation. In *Proceedings of the Scalable Parallel Libraries Conference, October 6–8, 1993, Mississippi State, Mississippi*, pages 160–165, 1109 Spring Street, Suite 300, Silver Spring, MD 20910, USA, 1994. IEEE Computer Society Press.

[42] W. Gropp and E. Lusk. Scalable Unix tools on parallel processors. In *Proceedings of the Scalable High-Performance Computing Conference, May 23–25, 1994, Knoxville, Tennessee*, pages 56–62, 1109 Spring Street, Suite 300, Silver Spring, MD 20910, USA, 1994. IEEE Computer Society Press.

[43] W. D. Gropp and B. F. Smith. Experiences with domain decomposition in three dimensions: overlapping Schwarz methods. In *Domain Decomposition Methods in Science and Engineering: The Sixth International Conference on Domain Decomposition*, volume 157 of *Contemporary Mathematics*, pages 323–333, Providence, Rhode Island, 1994. American Mathematical Society.

[44] L. Kettunen, K. Forsman, D. Levine, and William D. Gropp. Solutions of team problems 13 and 20 using a volume integral formulation. In *Proceedings of Aix-les-Bains TEAM workshop*, 1994.

[45] Kimmo Forsman, William Gropp, Lauri Kettunen, and David Levine. Computational electromagnetics and parallel dense matrix computations. In Bailey, David H., Bjørstad, Petter E., Gilbert, John E., Mascagni, Michael V., Schreiber, Robert S., Simon, Horst D., Torczon, Virginia J. and Layne T. Watson, editors, *Proceedings of the 27th Conference on Parallel Processing for Scientific Computing*, pages 225–230, Philadelphia, PA, USA, February15–17 1995. SIAM Press.

[46] W. D. Gropp, D. E. Keyes, and M. D. Tidriri. Parallel implicit solvers for steady, compressible aerodynamics. In *Parallel Computational Fluid Dynamics*, pages 391–399. Elsevier Science Publishers B.V. (North–Holland), Amsterdam, 1995.

[47] W. Gropp and E. Lusk. Dynamic process management in an MPI setting. In *Proceedings / Seventh IEEE Symposium on Parallel and Distributed Processing, October 25–28, 1995, San Antonio, Texas*, pages 530–534, 1109 Spring Street, Suite 300, Silver Spring, MD 20910, USA, 1995. IEEE Computer Society Press. IEEE catalog number 95TB8131.

[48] W. Gropp and E. Lusk. Implementing MPI: the 1994 MPI Implementors' Workshop. In *Proceedings of the 1994 Scalable Parallel Libraries Conference: October 12–14, 1994, Mississippi State University, Mississippi*, pages 55–59, 1109 Spring Street, Suite 300, Silver Spring, MD 20910, USA, 1995. IEEE Computer Society Press.

[49] W. Gropp, E. Karrels, and E. Lusk. MPE graphics: scalable X11 graphics in MPI. In *Proceedings of the 1994 Scalable Parallel Libraries Conference: October 12–14, 1994, Mississippi State University, Mississippi*, pages 49–54, 1109 Spring Street, Suite 300, Silver Spring, MD 20910, USA, 1995. IEEE Computer Society Press.

[50] William D. Gropp and Ewing L. Lusk. A taxonomy of programming models for symmetric multiprocessors and smp clusters. In W. K. Giloi, S. Jahnichen, and B. D. Shriver, editors, *Programming Models for Massively Parallel Computers*, pages 2–7. IEEE Computer Society Press, October 1995.

[51] William D. Gropp, Lois Curfman McInnes, and Barry Smith. Scalable libraries for solving systems of nonlinear equations and unconstrained minimization problems. In *Proceedings of the 1994 Scalable Parallel Libraries Conference: October 12–14, 1994, Mississippi State University, Mississippi*, pages 60–67, 1109 Spring Street, Suite 300, Silver Spring, MD 20910, USA, 1995. IEEE Computer Society Press.

[52] W. Gropp and E. Lusk. The MPI message-passing interface standard: Overview and status. In Grandinetti et al, editor, *High performance computing: technology, methods, and applications (Advanced workshop, June 1994, Cetraro, Italy)*, volume 10 of *Advances in Parallel Computing*, pages 265–270, Amsterdam, The Netherlands, 1995. Elsevier.

[53] William D. Gropp and Barry Smith. Parallel domain decomposition software. In D. E. Keyes, Youcef Saad, and Donald G. Truhlar, editors, *Domain-Based Parallelism and Problem Decomposition Methods in Computational Science and Engineering*. SIAM, Philadelphia, 1995.

[54] Rajeev Thakur, William Gropp, and Ewing Lusk. An abstract-device interface for implementing portable parallel-I/O interfaces. In *Proceedings of Frontiers '96: The Sixth Symposium on the Frontiers of Massively Parallel Computation*, pages 180–187, Annapolis, Maryland, October 27–31, 1996. IEEE Computer Society.

[55] A. Geist, W. Gropp, S. Huss-Lederman, A. Lumsdaine, E. Lusk, W. Saphir, T. Skjellum, and M. Snir. MPI-2: extending the Message-Passing Interface. In Luc Bouge, P. Fraigniaud, A. Mignotte, and Y. Robert, editors, *Euro-Par '96 parallel processing: second International Euro-Par Conference, Lyon, France, August 26–29, 1996: proceedings*, volume 1123–1124 of *Lecture notes in computer science*, pages 128–135, Berlin, Germany / Heidelberg, Germany / London, UK / etc., 1996. Springer-Verlag.

[56] William D. Gropp. Why we couldn't use numerical libraries for PETSc. In Ronald F. Boisvert, editor, *Proceedings of the IFIP TC2/WG2.5 Working Conference on the Quality of Numerical Software, Assessment and Enhancement*, pages 249–254. Chapman & Hall, 1997.

[57] Rajeev Thakur, William Gropp, and Ewing Lusk. An experimental evaluation of the parallel I/O systems of the IBM SP and Intel Paragon using a production application. In *Proceedings of the Third International Conference of the Austrian Center for Parallel Computation (ACPC)*, volume 1127 of *Lecture Notes in Computer Science*, pages 24–35. Springer-Verlag, September 1996.

[58] S. Balay, W. D. Gropp, L. C. McInnes, and B. F. Smith. Efficient management of parallelism in object-oriented numerical software libraries. In E. Arge, A. M. Bruaset, and H. P. Langtangen, editors, *Modern Software Tools in Scientific Computing*, pages 163–202. Birkhauser Press, 1997.

[59] William D. Gropp. An introduction to performance debugging for parallel computers. In D. Keyes, A. Sameh, and V. Venkatakrishnan, editors, *Parallel Numerical Algorithms*, pages 369–382. Kluwer Academic Publishers, 1997.

[60] W. Gropp and Jorge Mor. Optimization environments and the NEOS server. In M. D. Buhmann and A. Iserles, editors, *Approximation Theory and Optimization: Tributes to M. J. D. Powell*, pages 167–182. Cambridge University Press, 1997.

[61] William D. Gropp, D.E. Keyes, L.C. McInnes, and M.D. Tidriri. Parallel implicit PDE computations: Algorithms and software. In *Proceedings of Parallel CFD'97*, pages 333–344. Elsevier, 1997.

[62] William D. Gropp and Ewing Lusk. Why are PVM and MPI so different? In Marian Bubak, Jack Dongarra, and Jerzy Waśniewski, editors, *Recent Advances in Parallel Virtual Machine and Message Passing Interface*, volume 1332 of *Lecture Notes in Computer Science*, pages 3–10. Springer Verlag, 1997. 4th European PVM/MPI Users' Group Meeting, Cracow, Poland, November 1997.

[63] William D. Gropp. Performance driven programming models. In *Massively Parallel Programming Models (MPPM-97)*, pages 61–67. IEEE Computer Society Press, 1997. November 12-14, 1997; London; Third working conference.

[64] William D. Gropp. Which comes first: The architecture or the algorithm? (abstract). In A. Veidenbaum and K. Joe, editors, *Innovative Architectures for Future Generation High-Performance Processors and Systems*, page 13. IEEE Computer Society, 1998.

[65] Rajeev Thakur, William Gropp, and Ewing Lusk. Data sieving and collective I/O in ROMIO. In *Proceedings of the 7th Symposium on the Frontiers of Massively Parallel Computation*, pages 182–189. IEEE Computer Society Press, February 1999.

[66] William Gropp. Exploiting existing software in libraries: Successes, failures, and reasons why. In Michael Henderson, Christopher Anderson, and Stephen L. Lyons, editors, *Object Oriented Methods for Interoperable Scientific and Engineering Computing*, pages 21–29. SIAM, SIAM, 1999.

[67] Satish Balay, William Gropp, Lois Curfman McInnes, and Barry Smith. A microkernel design for component-based numerical software systems. In Michael Henderson, Christopher Anderson, and Stephen L. Lyons, editors, *Object Oriented Methods for Interoperable Scientific and Engineering Computing*, pages 60–69. SIAM, SIAM, 1998. Also ANL/MCS-P727-0998.

[68] Rajeev Thakur, Ewing Lusk, and William Gropp. A case for using MPI's derived datatypes to improve I/O performance. In *Proceedings of SC98: High Performance Networking and Computing*, November 1998.

[69] William Gropp, Ewing Lusk, and Debbie Swider. Improving the performance of MPI derived datatypes. In Anthony Skjellum, Purushotham V. Bangalore, and Yoginder S. Dandass, editors, *Proceedings of the Third MPI Developer's and User's Conference*, pages 25–30, Starkville, MS, 1999. MPI Software Technology Press.

[70] Rajeev Thakur, William Gropp, and Ewing Lusk. On implementing MPI-IO portably and with high performance. In *Proceedings of the 6th Workshop on I/O in Parallel and Distributed Systems*, pages 23–32. ACM Press, May 1999.

[71] W. D. Gropp, D. K. Kaushik, D. E. Keyes, and B. F. Smith. Towards realistic performance bounds for implicit CFD codes. In *Proceedings of Parallel CFD'99*, pages 241–248, 1999.

[72] William D. Gropp and Ewing Lusk. Reproducible measurements of MPI performance characteristics. In Jack Dongarra, Emilio Luque, and Tomàs Margalef, editors, *Recent Advances in Parallel Virtual Machine and Message Passing Interface*, volume 1697 of *Lecture Notes in Computer Science*, pages 11–18. Springer Verlag, 1999. 6th European PVM/MPI Users' Group Meeting, Barcelona, Spain, September 1999.

[73] James Cownie and William Gropp. A standard interface for debugger access to message queue information in MPI. In Jack Dongarra, Emilio Luque, and Tomàs Margalef, editors, *Recent Advances in Parallel Virtual Machine and Message Passing Interface*, volume 1697 of *Lecture Notes in Computer Science*, pages 51–58. Springer Verlag, 1999. 6th European PVM/MPI Users' Group Meeting, Barcelona, Spain, September 1999.

[74] W. K. Anderson, William D. Gropp, D. K. Kaushik, D. E. Keyes, and B. F. Smith. Achieving high sustained performance in an unstructured mesh CFD application. In *Proceedings of the ACM/IEEE SC99 Conference on High Performance Networking and Computing*. IEEE Computer Society, 1999. CDROM. Also at http://www.sc99.org and ICASE Report No. 2000-2.

[75] Lori A. Freitag, William Gropp, Paul D. Hovland, Lois C. McInnes, and Barry F. Smith. Infrastructure and interfaces for large-scale numerical software. In *Proceedings of PDPTA 1999*, pages 2657–2664, 1999.

[76] Nicholas T. Karonis, Bronis R. de Supinski, Ian Foster, William Gropp, Ewing Lusk, and John Bresnahan. Exploiting hierarchy in parallel computer networks to optimize collective operation performance. In *Fourteenth International Parallel and Distributed Processing Symposium*, pages 377–384, May 2000.

[77] R. Butler, W. Gropp, and E. Lusk. A scalable process-management environment for parallel programs. In Jack Dongarra, Peter Kacsuk, and Norbert Podhorszki, editors, *Recent Advances in Parallel Virutal Machine and Message Passing Interface*, number 1908 in Springer Lecture Notes in Computer Science, pages 168–175, September 2000.

[78] William D. Gropp. Runtime checking of datatype signatures in MPI. In Jack Dongarra, Peter Kacsuk, and Norbert Podhorszki, editors, *Recent Advances in Parallel Virutal Machine and Message Passing Interface*, number 1908 in Springer Lecture Notes in Computer Science, pages 160–167, September 2000. 7th European PVM/MPI Users' Group Meeting.

[79] W. D. Gropp, D. K. Kaushik, B. F. Smith, and D. E. Keyes. Analyzing the parallel scalablity of an implicit unstructured mesh CFD code. In Mateo Valero, Viktor K. Prasanna, and Sriram Vajapeyam, editors, *High Performance Computing – HiPC2000*, number 1970 in Lecture Notes in Computer Science, pages 395–404. Springer Verlag, 2000.

[80] William Gropp. Solving CFD problems with open source parallel libraries. In Tor Sorevik, Fredrik Manne, Randi Moe, and Assefaw Hadish Gebremedhin, editors, *Applied Parallel*

Computing: New Paradigms for HPC in Industry and Academia, number 1947 in Lecture Notes in Computer Science, page 52. Springer Verlag, 2000. (Abstract).

[81] C. Eric Wu, Anthony Bolmarcich, Marc Snir, David Wootton, Farid Parpia, Anthony Chan, Ewing L. Lusk, and William Gropp. From trace generation to visualization: A performance framework for distributed parallel systems. In *Proceedings of SC2000*.

[82] Kristopher R. Buschelman, William Gropp, Lois C. McInnes, and Barry F. Smith. PETSc and Overture: Lessons learned developing an interface between components. In *The Architecture of Scientific Software 2000*, pages 57–68, 2000.

[83] Alain Roy, Ian Foster, William Gropp, Nicholas Karonis, Volker Sander, and Brian Toonen. MPICH-GQ: Quality of service for message passing programs. In *Proceedings of SC2000*, 2000.

[84] Rajkumar Vinkat, Philip M. Dickens, and William Gropp. Efficient communication across the Internet in wide-area MPI. In *Proceedings of Parallel and Distributed Processing Techniques and Applications*, 2001.

[85] Brian Toonen, David Ashton, Ewing Lusk, Ian Foster, William Gropp, Edgar Gabriel, Ralph Butler, and Nicholas Karonis. Interfacing parallel jobs to process managers. In *Proceedings of the 10th IEEE International Symposium on High Performance Distributed Computing*, pages 431–432. IEEE Computer Society Press, August 2001.

[86] Eric Webb, Jay Alameda, William Gropp, Joshua Gray, and Richard Alkire. Performance of tightly coupled Linux cluster simulation using PETSc of reaction and transport processes during corrosion pit initiation. In *Proceedings of Linux Clusters: the HPC Revolution*, 2001. Urbana, IL.

[87] William Gropp. Advanced cluster programming with mpi. In *CLUSTER*, page 453. IEEE Computer Society, 2001.

[88] Emil Ong, Ewing Lusk, and William Gropp. Scalable Unix commands for parallel processors: A high-performance implementation. In Y. Cotronis and J. Dongarra, editors, *Recent Advances in Parallel Virtual Machine and Message Passing Interface*, volume 2131 of *Lecture Notes in Computer Science*, pages 410–418. Springer-Verlag, September 2001. 8th European PVM/MPI Users' Group Meeting.

[89] William Gropp. Challenges and successes in achieving the potential of mpi. In Y. Cotronis and J. Dongarra, editors, *Recent Advances in Parallel Virtual Machine and Message Passing Interface*, volume 2131 of *Lecture Notes in Computer Science*, page 7, September 2001.

[90] W. D. Gropp, D. K. Kaushik, D. E. Keyes, and B. F. Smith. Latency, bandwidth, and concurrent issue limitations in high-performance CFD. In *Proceedings of the First MIT Conference on Computational Fluid and Solid Mechanics*, June 2001.

[91] William D. Gropp. Learning from the success of MPI. In Burkhard Monien, Viktor K. Prasanna, and Sriram Vajapeyam, editors, *High Performance Computing – HiPC 2001*, number 2228 in Lecture Notes in Computer Science, pages 81–92. Springer, December 2001. 8th International Conference.

[92] Philip M. Dickens and William D. Gropp. An evaluation of a user-level data transfer mechanism for high-performance networks. In *Proceedings of HPDC'02*, pages 255–264, 2002.

[93] Philip M. Dickens, William Gropp, and Paul R. Woodward. High performance wide area data transfers over high performance networks. In *Proceedings of IPDPS 2002*, 2002.

[94] William D. Gropp and Ewing Lusk. Goals guiding design: PVM and MPI. In William Gropp, Rob Pennington, Dan Reed, Mark Baker, Maxine Brown, and Rajkumar Buyya, editors, *Proceedings of IEEE Cluster*, pages 257–265. IEEE Computer Society, 2002.

[95] Seongbok Baik, Cynthia S. Hood, and William D. Gropp. Prototype of AM3: Active mapper and monitoring module for Myrinet environment. In *HSLN (High-Speed Local Networks) workshop*, pages 703–707, 2002.

[96] A. Ching, A. Choudhary, W.-K. Liao, R. Ross, and W. Gropp. Noncontiguous I/O through PVFS. In William Gropp, Rob Pennington, Dan Reed, Mark Baker, Maxine Brown, and Rajkumar Buyya, editors, *Proceedings of IEEE Cluster*, pages 405–414. IEEE Computer Society, 2002.

[97] William D. Gropp. Building library components that can use any MPI implementation. In Dieter Kranzlmüller, Peter Kacsuk, Jack Dongarra, and Jens Volkert, editors, *Recent Advances in Parallel Virtual Machine and Message Passing Interface*, number LNCS2474 in Lecture Notes in Computer Science, pages 280–287. Springer Verlag, 2002. 9th European PVM/MPI Users' Group Meeting, Linz, Austria.

[98] William Gropp and Ewing L. Lusk. Mpi on the grid. In Dieter Kranzlmüller, Peter Kacsuk, Jack Dongarra, and Jens Volkert, editors, *Recent Advances in Parallel Virtual Machine and Message Passing Interface*, number LNCS2474 in Lecture Notes in Computer Science, page 12. Springer Verlag, 2002.

[99] William Gropp. Mpich2: A new start for mpi implementations. In Dieter Kranzlmüller, Peter Kacsuk, Jack Dongarra, and Jens Volkert, editors, *Recent Advances in Parallel Virtual Machine and Message Passing Interface*, number LNCS2474 in Lecture Notes in Computer Science, page 7. Springer Verlag, 2002.

[100] Jeffrey J. Evans, Seongbok Baik, Cynthia S. Hood, and William Gropp. Toward understanding soft faults in high performance cluster networks. In *Proceedings of the 8th IFIP/IEEE International Symposium on Integrated Network Management*, pages 117–120, March 2003.

[101] William Gropp. Trends in high performance computing. In *High Performance Computing with QCDOC and BlueGene*, volume 50, pages 91–97. RIKEN BNL Research Center, February 2003. Abstract and six major slides from the presentation.

[102] A. Ching, A. Choudhary, K. Coloma, W.-K. Liao, R. Ross, and W. Gropp. Noncontiguous I/O accesses through MPI-IO. In *Proceedings of the 3rd IEEE/ACM International Symposium on Cluster Computing and the Grid (CCGrid2003)*, pages 104–111, May 2003.

[103] William Gropp. Future developments in MPI. In Jack Dongarra, Domenico Laforenza, and Salvatore Orlando, editors, *Recent Advances in Parallel Virtual Machine and Message Passing Interface*, number LNCS2840 in Lecture Notes in Computer Science, pages 15–15. Springer Verlag, 2003. 10th European PVM/MPI User's Group Meeting, Venice, Italy.

[104] Rajeev Thakur and William Gropp. Improving the performance of collective operations in MPICH. In Jack Dongarra, Domenico Laforenza, and Salvatore Orlando, editors, *Recent Advances in Parallel Virtual Machine and Message Passing Interface*, number LNCS2840 in

Lecture Notes in Computer Science, pages 257–267. Springer Verlag, 2003. 10th European PVM/MPI User's Group Meeting, Venice, Italy.

[105] G. Almási, C. Archer, J. G. Casta nos, M. Gupta, X. Martorell, J. E. Moreira, W. D. Gropp, S. Rus, and B. Toonen. MPI on BlueGene/L: Designing an efficient general purpose messaging solution for a large cellular system. In Jack Dongarra, Domenico Laforenza, and Salvatore Orlando, editors, *Recent Advances in Parallel Virtual Machine and Message Passing Interface*, number LNCS2840 in Lecture Notes in Computer Science, pages 352–361. Springer Verlag, 2003. 10th European PVM/MPI User's Group Meeting, Venice, Italy.

[106] R. Ross, N. Miller, and W. D. Gropp. Implementing fast and reusable datatype processing. In Jack Dongarra, Domenico Laforenza, and Salvatore Orlando, editors, *Recent Advances in Parallel Virtual Machine and Message Passing Interface*, number LNCS2840 in Lecture Notes in Computer Science, pages 404–413. Springer Verlag, 2003. 10th European PVM/MPI User's Group Meeting, Venice, Italy.

[107] William Gropp and Ewing L. Lusk. High-level programming in mpi. In Jack Dongarra, Domenico Laforenza, and Salvatore Orlando, editors, *Recent Advances in Parallel Virtual Machine and Message Passing Interface*, number LNCS2840 in Lecture Notes in Computer Science, page 27. Springer Verlag, 2003.

[108] Jeffrey Evans, Cynthia Hood, and William Gropp. Exploring the relationship between parallel application run-time variability and network performance. In *Workshop on High-Speed Local Networks (HSLN), IEEE Conference on Local Computer Networks (LCN)*, pages 538–547, October 2003.

[109] J. Li, W. Liao, A. Choudhary, R. Ross, R. Thakur, W. Gropp, R. Latham, A. Siegel, B. Gallagher, and M. Zingale. Parallel netCDF: A high-performance scientific I/O interface. In *Proceedings of SC2003*, November 2003.

[110] A. Ching, A. Choudhary, W.-K. Liao, R. Ross, and W. Gropp. Efficient structured data access in parallel file systems. In *Proceedings of IEEE Cluster*. IEEE Computer Society, November 2003.

[111] George Almasi, Charles Archer, Jose G. Castanos, C. Chris Erway, Philip Heidelberger, Xavier Martorell, Jose E. Moreira, Kurt Pinnow, Joe Ratterman, Nils Smeds, Burkhard Steinmacher-Burow, William Gropp, and Brian Toonen. Implementing MPI on the Blue-Gene/L supercomputer. In *Proceedings of EuroPar2004*, pages 833–845, 2004. Selected as distinquished paper.

[112] William Gropp. MPI and high productivity programming. In Dieter Kranzlmüller, Peter Kacsuk, and Jack Dongarra, editors, *Recent Advances in Parallel Virtual Machine and Message Passing Interface*, number LNCS3241 in Lecture Notes in Computer Science, page 7. Springer Verlag, 2004. 11th European PVM/MPI User's Group Meeting, Budapest, Hungary.

[113] Rajeev Thakur, William Gropp, and Brian Toonen. Minimizing synchronization overhead in the implementation of MPI one-sided communication. In Dieter Kranzlmüller, Peter Kacsuk, and Jack Dongarra, editors, *Recent Advances in Parallel Virtual Machine and Message Passing Interface*, number LNCS3241 in Lecture Notes in Computer Science, pages 57–67. Springer Verlag, 2004. 11th European PVM/MPI User's Group Meeting, Budapest, Hungary.

[114] W. Jiang, J. Liu, H.-W. Jin, D. K. Panda, D. Buntinas, Rajeev Thakur, and William Gropp. Efficient implementation of MPI-2 passive one-sided communication on InfiniBand clusters. In Dieter Kranzlmüller, Peter Kacsuk, and Jack Dongarra, editors, *Recent Advances in Parallel Virtual Machine and Message Passing Interface*, number LNCS3241 in Lecture Notes in Computer Science, pages 68–76. Springer Verlag, 2004. 11th European PVM/MPI User's Group Meeting, Budapest, Hungary.

[115] Jiuxing Liu, Weihang Jiang, Pete Wyckoff, Dhabaleswar K. Panda, David Ashton, Darius Buntinas, William Gropp, and Brian Toonen. Design and implementation of MPICH2 over Infiniband with RDMA support. In *Proceedings of IPDPS 2004*, 2004.

[116] William Gropp, Robert Ross, and Neill Miller. Providing efficient I/O redundancy in MPI environments. In Dieter Kranzlmüller, Peter Kacsuk, and Jack Dongarra, editors, *Recent Advances in Parallel Virtual Machine and Message Passing Interface*, number LNCS3241 in Lecture Notes in Computer Science, pages 77–86. Springer Verlag, 2004. 11th European PVM/MPI User's Group Meeting, Budapest, Hungary.

[117] William D. Gropp. Mpi and high productivity programming. In *PVM/MPI*, page 7, 2004.

[118] Chris Falzone, Anthony Chan, Ewing Lusk, and William Gropp. Collective error detection for MPI collective operations. In Beniamino Di Martino, Dieter Kranzluüller, and Jack Dongarra, editors, *Recent Advances in Parallel Virtual Machine and Message Passing Interface*, number LNCS 3666 in Lecture Notes in Computer Science, pages 138–147. Springer Verlag, September 2005. 12th European PVM/MPI User's Group Meeting, Sorrento, Italy.

[119] Darius Buntinas and William Gropp. Designing a common communication subsystem. In Beniamino Di Martino, Dieter Kranzluüller, and Jack Dongarra, editors, *Recent Advances in Parallel Virtual Machine and Message Passing Interface*, number LNCS 3666 in Lecture Notes in Computer Science, pages 156–166. Springer Verlag, September 2005. 12th European PVM/MPI User's Group Meeting, Sorrento, Italy.

[120] William Gropp and Rajeev Thakur. An evaluation of implementation options for MPI one-sided communication. In Beniamino Di Martino, Dieter Kranzluüller, and Jack Dongarra, editors, *Recent Advances in Parallel Virtual Machine and Message Passing Interface*, number LNCS 3666 in Lecture Notes in Computer Science, pages 415–424. Springer Verlag, September 2005. 12th European PVM/MPI User's Group Meeting, Sorrento, Italy.

[121] William Gropp. Towards a productive MPI environment (abstract). In Beniamino Di Martino, Dieter Kranzluüller, and Jack Dongarra, editors, *Recent Advances in Parallel Virtual Machine and Message Passing Interface*, number LNCS 3666 in Lecture Notes in Computer Science, page 4. Springer Verlag, September 2005. 12th European PVM/MPI User's Group Meeting, Sorrento, Italy.

[122] Ernie Chan, William Gropp, Rajeev Thakur, and Robert van de Geijn. Collective communication on architectures that support simultaneous communication over multiple links. In *Proceedings of the 2006 ACM SIGPLAN Symposium on Principles and Practice of Parallel Programming*, pages 2–11, New York, New York, USA, March 29-31 2006. ACM.

[123] Dariums Buntinas, Guillaume Mercier, and William Gropp. Design and evaluation of Nemesis, a scalable, low-latency, message-passing communication subsystem. In Stephen John Turner, Bu Sung Lee, and Wentong Cai, editors, *Proceedings of the 6th IEEE International Symposium on Cluster Computing and the Grid (CCGrid2006)*, pages 521–530, May 2006.

[124] William D. Gropp and Rajeev Thakur. Issues in developing a thread-safe MPI implementation. In Bernd Mohr, Jesper Larsson Träff, Joachim Worringen, and Jack Dongarra, editors, *Recent Advances in Parallel Virtual Machine and Message Passing Interface*, number LNCS 4192 in Springer Lecture Notes in Computer Science, pages 12–21. Springer, September 2006.

[125] Salman Pervez, Ganesh Gopalakrishnan, Robert M. Kirby, Rajeev Thakur, and William D. Gropp. Formal verification of programs that use MPI one-sided communication. In Bernd Mohr, Jesper Larsson Träff, Joachim Worringen, and Jack Dongarra, editors, *Recent Advances in Parallel Virtual Machine and Message Passing Interface*, number LNCS 4192 in Springer Lecture Notes in Computer Science, pages 30–39. Springer, September 2006.

[126] Christopher Gottbrath, Brian Barrett, William D. Gropp, Ewing "Rusty" Lusk, and Jeff Squyres. An interface to support the identification of dynamic MPI 2 processes for scalable parallel debugging. In Bernd Mohr, Jesper Larsson Träff, Joachim Worringen, and Jack Dongarra, editors, *Recent Advances in Parallel Virtual Machine and Message Passing Interface*, number LNCS 4192 in Springer Lecture Notes in Computer Science, pages 115–122. Springer, September 2006.

[127] Surendra Byna, Xian-He Sun, Rajeev Thakur, and William D. Gropp. Automatic memory optimization for improving MPI derived datatype performance. In Bernd Mohr, Jesper Larsson Träff, Joachim Worringen, and Jack Dongarra, editors, *Recent Advances in Parallel Virtual Machine and Message Passing Interface*, number LNCS 4192 in Springer Lecture Notes in Computer Science, pages 238–246. Springer, September 2006.

[128] William D. Gropp, Dinesh K. Kaushik, David E. Keyes, and Barry F. Smith. Parallel implicit solution of diffusion-limited radiation transport. In Olof B. Widlund and David E. Keyes, editors, *Domain Decomposition Methods in Science and Engineering XVI*, volume 55 of *Lecture Notes in Computational Science and Engineering*, pages 579–586. Springer-Verlag, 2006.

6 Technical Reports

[1] J. H. Bolstad, T. F. Chan, W. M. Coughran, Jr., W. D. Gropp, E. H. Grosse, M. T. Heath, R. J. LeVeque, F. T. Luk, S. G. Nash, and L. N. Trefethen. Numerical analysis program library user's guide (NAPLUG). User Note 82, SLAC Computing Services, 1979. First issued in 1976 by Chan, Coughran, Heath, and Luk.

[2] William D. Gropp. Numerical solution of transport equations. Technical Report STAN-CS-81-888, Stanford University, December 1981. Ph.D. Thesis.

[3] William D. Gropp. Local uniform mesh refinement for elliptic partial differential equations. Technical Report YALE/DCS/RR-278, Yale University, Department of Computer Science, July 1983.

[4] G. W. Hedstrom and William D. Gropp. The computer as an aid in the asymptotic estimation of integrals. Technical Report UCRL-87297, Lawrence Livermore National Laboratory, August 1983.

[5] W. D. Gropp, J. J. O'Donnell, S. T. O'Donnell, M. H. Schultz, and B. Weston. A high performance bulk memory system. Technical Report YALE/DCS/RR-311, Yale University, Department of Computer Science, March 1984.

[6] W. D. Gropp. Local uniform mesh refinement with moving grids. Technical Report YALEU/DCS/RR-313, Yale University, April 1984.

[7] W. D. Gropp. Local uniform mesh refinement on loosely-coupled parallel processors. Technical Report YALEU/DCS/RR-352, Yale University, December 1984.

[8] D. E. Keyes and W. D. Gropp. A comparison of domain decomposition techiques for elliptic partial differential equations and their parallel implementation. Techical Report YALEU/DCS/RR-448, Comput. Sci. Dept., Yale Univ., December 1985.

[9] W. Gropp. Dynamic grid manipulation for PDE's on hypercube parallel processors. Technical Report YALEU/DCS/RR-458, Department of Computer Science, Yale University, March 1986.

[10] W. D. Gropp and E. B. Smith. Computational fluid dynamics on parallel processors. Technical Report YALEU/DCS/RR-570, Department of Computer Science, Yale University, December 1987.

[11] R. H. Herbin, W. D. Gropp, D. E. Keyes, and V. Sonnad. A domain decomposition technique on a loosely coupled array of processors. Technical Report KGN-124, IBM Kingston, 1987.

[12] W. Gropp and I. Ipsen. Recursive mesh refinement on hypercubes. Technical Report YALE/DCS/RR-616, Department of Computer Science , Yale University, March 1988.

[13] L. Greengard and W. Gropp. A parallel version of the fast multipole method. Technical Report YALE/DCS/RR-640, Yale University, Department of Computer Science, August 1988.

[14] H. Berryman, J. Saltz, W. Gropp, and R. Mirchandaney. Krylov methods preconditioned with incompletely factored matrices on the CM-2. Technical Report 89-54, NASA Langley Research Center, ICASE, Hampton, VA, December 1989. Also Yale University YALE/DCS/RR-685, March 1989.

[15] William D. Gropp and David Keyes. Domain decomposition on parallel computers. Technical Report YALE/DCS/RR-723, Yale University, Department of Computer Science, August 1989.

[16] David E. Keyes and William D. Gropp. Domain decomposition with local mesh refinement. Technical Report YALEU/DCS/RR-726, Yale University, August 1989.

[17] William D. Gropp and David Keyes. Parallel performance of domain-decomposed preconditioned Krylov methods for PDEs with adaptive refinement. Technical Report YALE/DCS/RR-773, Yale University, Department of Computer Science, April 1990. Also ANL Preprint MCS-P147-0490, May 1990.

[18] William D. Gropp and David E. Keyes. Parallel domain decomposition and the solution of non-linear systems of equations. Technical Report MCS-P186-1090, Mathematics and Computer Science Division, Argonne National Laboratory, November 1990.

[19] David E. Keyes and William D. Gropp. Domain-decomposable preconditioners for second-order upwind discretizations of multicomponent systems. Technical Report MCS-187-1090, Mathematics and Computer Science Division, Argonne National Laboratory, November 1990.

[20] X.-C. Cai, William D. Gropp, and David E. Keyes. Convergence rate estimate for a domain decomposition method. Technical Report YALE/DCS/RR-827, Yale University, Department of Computer Science, January 1991. also ANL Preprint MCS-P202-1290, January 1991.

[21] William D. Gropp and David E. Keyes. Domain decomposition with local mesh refinement. Technical Report 91-19, ICASE, February 1991.

[22] William D. Gropp and David E. Keyes. Domain decomposition methods in computational fluid dynamics. Technical Report 91-20, ICASE, February 1991. Also ANL Preprint MCS-P210-0191, April 1991.

[23] William D. Gropp. Parallel computing and domain decomposition. Technical Report MCS-P257-0891, Mathematics and Computer Science Division, Argonne National Laboratory, September 1991.

[24] William Gropp and Ewing Lusk. A test implementation of the MPI draft message-passing standard. Technical Report ANL-92/47, Mathematics and Computer Science Division, Argonne National Laboratory, December 92.

[25] William D. Gropp and Barry F. Smith. Experiences with domain decomposition in three dimensions: Overlapping Schwarz methods. Technical report, Mathematics and Computer Science Division, Argonne National Laboratory, 1992. Appeared in the Proceedings of the Sixth International Symposium on Domain Decomposition Methods.

[26] David E. Keyes and William D. Gropp. Domain decomposition as a mechanism for using asymptotic methods. Technical Report MCS-P322-0892, Mathematics and Computer Science Division, Argonne National Laboratory, September 1992.

[27] William Gropp (ed.). Early experiences with the IBM SP-1. Technical Report ANL-MCS-TM-177, Mathematics and Computer Science Division, Argonne National Laboratory, May 1993.

[28] William Gropp. Early experiences with the IBM SP1 and the high-performance switch. Technical Report ANL-93/41, Mathematics and Computer Science Division, Argonne National Laboratory, November 93.

[29] William D. Gropp and Barry F. Smith. The design of data-structure-neutral libraries for the iterative solution of sparse linear systems. Technical Report MCS-P356-0393, Argonne National Laboratory, Argonne, IL, USA, March 1993.

[30] William D. Gropp, Hans Kaper, G. Leaf, D. Levine, V. Vinokur, and M. Palumbo. Numerical simulation of vortex dynamics in high-t_c superconductors. Technical Report MCS-P476-1094, Mathematics and Computer Science Division, Argonne National Laboratory, November 1994.

[31] L. Kettunen, K. Forsman, D. Levine, and W. Gropp. Integral equations in nonlinear 3d magnetostatics. Technical Report MCS-P460-0894, Mathematics and Computer Science Division, Argonne National Laboratory, August 1994.

[32] Anthony Skjellum, Ewing Lusk, and William Gropp. Early applications in the message passing interface (MPI). Technical report, Department of Computer Science, Mississippi State University, June 1994.

[33] William Gropp. An introduction to performance debugging for parallel computers. Technical Report MCS-P500-0295, Argonne National Lab, April 1995.

[34] William D. Gropp, Lois Curfman McInnes, and Barry F. Smith. Using the scalable nonlinear equations solvers package. Technical Memorandum ANL/MCS-TM-193, Argonne National Lab, February 1995.

[35] K. Forsman, W. Gropp, L. Kettunen, D. Levine, and J. Salonen. Solution of dense systems of linear equations arising from integral equation formulations. Technical Report MCS-P538-0895, Mathematics and Computer Science Division, Argonne National Laboratory, October 1995.

[36] Rajeev Thakur, Ewing Lusk, and William Gropp. I/O characterization of a portable astrophysics application on the IBM SP and Intel Paragon. Technical Report MCS-P534-0895, Mathematics and Computer Science Division, Argonne National Laboratory, August 1995. Revised October 1995.

[37] Rajeev Thakur, William Gropp, and Ewing Lusk. An experimental evaluation of the parallel I/O systems of the IBM SP and Intel Paragon using a production application. Technical Report MCS-P569–0296, Argonne National Laboratory, February 1996.

[38] Rajeev Thakur, William Gropp, and Ewing Lusk. An abstract-device interface for implementing portable parallel-I/O interfaces. Technical Report MCS-P592-0596, Argonne National Laboratory, Mathematics and Computer Science Division, May 1996.

[39] William D. Gropp and Jorge Moré. Optimization environments and the NEOS server. Technical Report ANL/MCS-P654-0397, Mathematics and Computer Science Division, Argonne National Laboratory, March 1997. Also CRPC-TR97708 and available at http://www.crpc.rice.edu/CRPC/softlib/TRs_online.html.

[40] William D. Gropp and Ewing Lusk. Why are PVM and MPI so different? Technical Report ANL/MCS-P667-0697, Mathematics and Computer Science Division, Argonne National Laboratory, June 1997.

[41] Rajeev Thakur, Ewing Lusk, and William Gropp. I/O in parallel applications: The weakest link. Technical Report ANL/MCS-P700-1197, Mathematics and Computer Science Division, Argonne National Laboratory, November 1997. Appeared in IJSA.

[42] Rajeev Thakur, Ewing Lusk, and William Gropp. A case for using MPI's derived datatypes to improve I/O performance. Technical Report ANL/MCS-P717-0598, Mathematics and Computer Science Division, Argonne National Laboratory, May 1998. Appeared at Supercomputing'98.

[43] Rajeev Thakur, William Gropp, and Ewing Lusk. Data sieving and collective I/O in ROMIO. Technical Report ANL/MCS-P723-0898, Mathematics and Computer Science Division, Argonne National Laboratory, August 1998. Submitted to Frontiers'99.

[44] Satish Balay, William Gropp, Lois Curfman McInnes, and Barry Smith. A microkernel design for component-based numerical software systems. Technical Report ANL/MCS-P727-0998, Mathematics and Computer Science Division, Argonne National Laboratory, September 1998.

[45] William Gropp, David E. Keyes, Lois C. McInnes, and M. D. Tidriri. Globalized Newton-Krylov-Schwarz algorithms and software for parallel implicit CFD. Technical Report 98-24, ICASE, August 1998. Also NASA/CR-1998-208435.

[46] Rajeev Thakur, William Gropp, and Ewing Lusk. Achieving high performance with MPI-IO. Technical Report ANL/MCS-P742-0299, Mathematics and Computer Science Division, Argonne National Laboratory, September 1999.

[47] Lori Freitag, William Gropp, Paul Hovland, Lois Curfman McInnes, and Barry Smith. Infrastructure and interfaces for large-scale numerical software. Technical Report ANL/MCS-P751-0599, Mathematics and Computer Science Division, Argonne National Laboratory, May 1999.

[48] William Gropp and Ewing Lusk. Reproducible measurements of MPI performance characteristics. Technical Report ANL/MCS-P755-0699, Mathematics and Computer Science Division, Argonne National Laboratory, June 1999.

[49] James Cownie and William Gropp. A standard interface for debugger access to message queue information in MPI. Technical Report ANL/MCS-P754-0699, Mathematics and Computer Science Division, Argonne National Laboratory, June 1999.

[50] Omer Zaki, Ewing Lusk, William Gropp, and Deborah Swider. Toward scalable performance visualization with Jumpshot. Technical Report ANL/MCS-P763-0699, Mathematics and Computer Science Division, Argonne National Laboratory, June 1999.

[51] W. Kyle Anderson, William D. Gropp, Dinesh Kaushik, David E. Keyes, and Barry F. Smith. Achieving high sustained performance in an unstructured mesh CFD applicatoin. Technical Report ANL/MCS-P776-0899, Mathematics and Computer Science Division, Argonne National Laboratory, August 1999. Appeared in Proceedings of SC99.

[52] William Gropp, David Keyes, Lois McInnes, and M. D. Tidiri. Globalized Newton-Krylov-Schwarz algorithms and software for parallel implicit CFD. Technical Report ANL/MCS-P788-0100, Mathematics and Computer Science Division, Argonne National Laboratory, January 2000. Appeared in High Performance Computing Applications.

[53] N. T. Karonis, B. R. de Supinski, I. Foster, W. Gropp, E. Lusk, and J. Bresnahan. Exploiting hierarchy in parallel computer networks to optimize collective operation performance. Technical Report ANL/MCS-P788-0200, Mathematics and Computer Science Division, Argonne National Laboratory, February 2000.

[54] William D. Gropp. Runtime checking of datatype signatures in MPI. Technical Report ANL/MCS-P826-0500, Mathematics and Computer Science Division, Argonne National Laboratory, May 2000.

[55] Ralph Butler, William Gropp, and Ewing Lusk. A scalable process-management environment for parallel programs. Technical Report ANL/MCS-P812-0400, Mathematics and Computer Science Division, Argonne National Laboratory, April 2000.

[56] William D. Gropp, Dinesh K. Kaushik, David E. Keyes, and Barry F. Smith. Performance modeling and tuning of an unstructured mesh CFD application. Technical Report ANL/MCS-P833-0700, Mathematics and Computer Science Division, Argonne National Laboratory, July 2000.

[57] Satish Balay, William Gropp, Lois Curfman McInnes, and Barry F. Smith. Software for the scalable solution of PDEs. Technical Report ANL/MCS-P834-0700, Mathematics and Computer Science Division, Argonne National Laboratory, July 2000.

[58] Rajeev Thakur and William Gropp. Parallel I/O. Technical Report ANL/MCS-P837-0700, Mathematics and Computer Science Division, Argonne National Laboratory, July 2000.

[59] Alain Roy, Ian Foster, William Gropp, Nicholas Karonis, Volker Sander, and Brian Toonen. MPICH-GQ: Quality of service for message passing programs. Technical Report ANL/MCS-P838-0700, Mathematics and Computer Science Division, Argonne National Laboratory, July 2000.

[60] W. D. Gropp, D. K. Kaushik, D. E. Keyes, and B. F. Smith. Understanding the parallel scalability of an implicit unstructured mesh CFD code. Technical Report ANL/MCS-P845-0900, Mathematics and Computer Science Division, Argonne National Laboratory, September 2000.

[61] W. D. Gropp, D. K. Kaushik, D. E. Keyes, and B. F. Smith. Latency, bandwidth, and concurrent issue limitations in high-performance CFD. Technical Report ANL/MCS-P850-1000, Mathematics and Computer Science Division, Argonne National Laboratory, October 2000.

[62] W. D. Gropp, D. K. Kaushik, D. E. Keyes, and B. F. Smith. High performance parallel implicit CFD. Technical Report ANL/MCS-P863-1200, Mathematics and Computer Science Division, Argonne National Laboratory, December 2000.

[63] Ralph Butler, William Gropp, and Ewing Lusk. Components and interfaces of a process management system for parallel programs. Technical Report ANL/MCS-P872-0201, Mathematics and Computer Science Division, Argonne National Laboratory, 2001.

[64] Emil Ong, Ewing Lusk, and William Gropp. Scalable Unix commands for parallel processors: A high-performance implementation. Technical Report ANL/MCS-P885-0601, Mathematics and Computer Science Division, Argonne National Laboratory, 2001.

[65] William Gropp. Learning from the success of MPI. Technical Report ANL/MCS-P903-0801, Mathematics and Computer Science Division, Argonne National Laboratory, 2001.

[66] William Gropp. Building library components that can use any MPI implementation. Technical Report ANL/MCS-P956-0502, Mathematics and Computer Science Division, Argonne National Laboratory, 2002.

[67] Anthony Chan, William Gropp, and Ewing Lusk. Scalable log files for parallel program trace data. Technical Report ANL/MCS-TM-256, Mathematics and Computer Science Division, Argonne National Laboratory, 2002.

[68] Nicholas T. Karonis, Bronis de Supinski, Ian Foster, William Gropp, Ewing Lusk, and Sebastien Lacour. A multilevel approach to topology-aware collective operations in computational grids. Technical Report ANL/MCS-P948-0402, Mathematics and Computer Science Division, Argonne National Laboratory, April 2002.

[69] Surendra Byna, William Gropp, Xian-He Sun, and Rajeev Thakur. Improving the performance of mpi derived datatypes by optimizing memory-access cost. Technical Report ANL/MCS-P1045-0403, Mathematics and Computer Science Division, Argonne National Laboratory, 2003.

[70] A. S. Bland, J. J. Dongarra, J. B. Drake, Jr. T. H. Dunigan, Jr. T. H. Dunning, A. Geist, B. Gorda, W. D. Gropp, R. J. Harrison, R. Kendall, D. Keyes, J. A. Nichols, L. Oliker, H. Simon, R. Stevens, III J. B. White, P. H. Worley, and T. Zacharia. Cray X1 evaluation. Technical Report ORNL/TM-2003/67, Oak Ridge National Laboratory, March 2003.

[71] Rajeev Thakur and William Gropp. Improving the performance of collective operations in MPICH. Technical Report ANL/MCS-P1038-0403, Mathematics and Computer Science Division, Argonne National Laboratory, 2003. Appeared in Euro PVMMPI'03.

[72] R. Ross, N. Miller, and W. D. Gropp. Implementing fast and reusable datatype processing. Technical Report ANL/MCS-P1068-0703, Mathematics and Computer Science Division, Argonne National Laboratory, July 2003. Appeared in Euro PVMMPI'03.

[73] Jiuxing Liu, Weihang Jiang, Pete Wyckoff, Dhabaleswar K. Panda, David Ashton, Darius Buntinas, William Gropp, and Brian Toonen. Design and implementation of MPICH2 over Infiniband with RDMA support. Technical Report ANL/MCS-P1103-1003, Mathematics and Computer Science Division, Argonne National Laboratory, 2003.

[74] Weihang Jiang, Jiuxing Liu, Hyun-Wook Jin, Dhabaleswar K. Panda, William Gropp, and Rajeev Thakur. High performance MPI-2 one-sided communication over InfiniBand. Technical Report ANL/MCS-P1119-0104, Mathematics and Computer Science Division, Argonne National Laboratory, 2004.

[75] Avery Ching, Alok Choudhary, Wei keng Liao, Robert Ross, and William Gropp. Evaluating structured I/O methods for parallel file systems. Technical Report ANL/MCS-P1125-0204, Mathematics and Computer Science Division, Argonne National Laboratory, 2004. To appear in IJHPCA.

[76] Rajeev Thakur, Rolf Rabenseifner, and William Gropp. Optimization of collective communication operations in MPICH. Technical Report ANL/MCS-P1140-0304, Mathematics and Computer Science Division, Argonne National Laboratory, March 2004.

[77] William Gropp and Ewing Lusk. Fault tolerance in MPI programs. Technical Report ANL/MCS-P1154-0404, Mathematics and Computer Science Division, Argonne National Laboratory, 2004.

[78] Rajeev Thakur, William Gropp, and Brian Toonen. Minimizing synchronization overhead in the implementation of MPI one-sided communication. Technical Report ANL/MCS-P1158-0504, Mathematics and Computer Science Division, Argonne National Laboratory, May 2004.

[79] Weihang Jiang, Kiuxing Liu, Hyun-Wook Jin, Dhabaleswar K. Panda, Darius Buntinas, Rajeev Thakur, and William Gropp. Efficient implementation of MPI-2 passive one-sided communication on InfiniBand clusters. Technical Report ANL/MCS-P1164-0504, Mathematics and Computer Science Division, Argonne National Laboratory, May 2004.

[80] William Gropp, Robert Ross, and Neill Miller. Providing efficient I/O redundancy in MPI environments. Technical Report ANL/MCS-P1178-0604, Mathematics and Computer Science Division, Argonne National Laboratory, June 2004.

[81] George Almási, Charles Archer, José G. Casta nos, John Gunnels, Chris Erway, Philip Heidelberger, Xavier Martorell, José E. Moreira, Kurt Pinnow, Joe Ratterman, Burkhard Steinmacher-burow, William Gropp, and Brian Toonen. The design and implementation of

message passing services for the BlueGene/L supercomputer. Technical Report ANL/MCS-P1183-0604, Mathematics and Computer Science Division, Argonne National Laboratory, June 2004.

[82] William D. Gropp. Issues in accurate and reliable use of parallel computing in numerical programs. Technical Report ANL/MCS-P1193-0804, Mathematics and Computer Science Division, Argonne National Laboratory, August 2004.

[83] Rajeev Thakur, William Gropp, and Brian Toonen. Optimizing the synchronization operations in MPI one-sided communication. Technical Report ANL/MCS-P1232-0205, Mathematics and Computer Science Division, Argonne National Laboratory, February 2005.

[84] Robert Ross, Robert Latham, William Gropp, Rajeev Thakur, and Brian Toonen. Implementing MPI-IO atomic mode without file system support. Technical Report ANL/MCS-P1235-0305, Mathematics and Computer Science Division, Argonne National Laboratory, March 2005.

[85] Darius Buntinas and William Gropp. Understanding the requirements imposed by programming model middleware on a common communication subsystem. Technical Report ANL/MCS-TM-284, Argonne National Laboratory, 2005.

[86] Darius Buntinas, Guillaume Mercier, and William Gropp. The design and evaluation of Nemesis, a scalable low-latency message-passing communication subsystem. Technical Report ANL/MCS-TM-292, Argonne National Laboratory, 2005.

[87] Darius Buntinas, Guillaume Mercier, and William Gropp. Data transfers between processes in an SMP system: Performance study and application to MPI. Technical Report ANL/MCS-P1306-1105, Argonne National Laboratory, 2005. Submitted to International Conference on Parallel and Processing (ICPP) 2006.

[88] William Gropp and Andrew Lumsdaine. Parallel tools and environments: A survey. Technical Report ANL/MCS-P1342-0406, Argonne National Laboratory, 2006. To appear in a SIAM volume of work presented at the SIAM Parallel Processing Conference in 2004.

[89] Boyana Norris, Albert Hartono, and William Gropp. Annotations for productivity and performance portability. Technical Report ANL/MCS-P1392-0107, Argonne National Laboratory, February 2007.

7 Manuals

[1] William D. Gropp and Barry Smith. *Simplified Linear Equation Solvers Users' Manual*. Argonne, IL, February 1993. ANL/MCS-93/8.

[2] William D. Gropp and Barry Smith. *Users Manual for the Chameleon Parallel Programming Tools*. Mathematics and Computer Science Division, Argonne National Laboratory, June 1993. ANL-93/23.

[3] William D. Gropp and Barry Smith. *Users Manual for KSP: Data-Structure-Neutral Codes Implementing Krylov Space Methods*. Mathematics and Computer Science Division, Argonne National Laboratory, August 1993. ANL-93/30.

[4] William D. Gropp, Ewing Lusk, and Steven Pieper. *Users Guide for the ANL IBM SP1.* Mathematics and Computer Science Division, Argonne National Laboratory, October 1994. ANL/MCS-TM-198.

[5] William D. Gropp and Ewing Lusk. *Users Guide for the ANL IBM SPx.* Mathematics and Computer Science Division, Argonne National Laboratory, December 1994. ANL/MCS-TM-199.

[6] William D. Gropp. *Users Manual for doctext: Producing Documentation from C Source Code.* Mathematics and Computer Science Division, Argonne National Laboratory, March 1995. ANL/MCS-TM 206.

[7] William D. Gropp. *Users Manual for tohtml: Producing True Hypertext Documents from LaTeX.* Mathematics and Computer Science Division, Argonne National Laboratory, March 1995. ANL/MCS-TM 207.

[8] William D. Gropp. *Users Manual for bfort: Producing Fortran Interfaces to C Source Code.* Mathematics and Computer Science Division, Argonne National Laboratory, March 1995. ANL/MCS-TM 208.

[9] William D. Gropp and Ewing Lusk. *Installation Guide for* `mpich`*, a Portable Implementation of MPI.* Mathematics and Computer Science Division, Argonne National Laboratory, 1996. ANL-96/5.

[10] William D. Gropp and Ewing Lusk. *User's Guide for* `mpich`*, a Portable Implementation of MPI.* Mathematics and Computer Science Division, Argonne National Laboratory, 1996. ANL-96/6.

[11] Satish Balay, William Gropp, Lois Curfman McInnes, and Barry Smith. *PETSc 2.0 Users Manual.* Mathematics and Computer Science Division, Argonne National Laboratory, 1997. ANL-95/11.

[12] Rajeev Thakur, William Gropp, and Ewing Lusk. *Users Guide for ROMIO: A High-Performance, Portable MPI-IO Implementation.* Mathematics and Computer Science Division, Argonne National Laboratory, October 1997. ANL/MCS-TM-234.

8   Recent Invited Talks

MPI and High Productivity Programming, invited colloquia at Ohio State University, Columbus, OH, February 8, 2007.

MPI: The Last Large Scale Success, invited presentation at Workshop on Programming Languages for High Performance Computing (HPC WPL). Also presented A Realistic Future as part of a panel on parallel programming directions, and a Programming Models Summary providing a summary of the workshop.

Overcoming the Barriers to Sustained Petaflop Performance, invited presentation at RWTH Aachen University of Technology, December, 2006. Also presented at Research Center Juelich, December, 2006.

Half Full or Half Empty, invited panel presentation for Thomas Sterling's multicore panel at Supercomputing 2006, November 2006.

Overcoming the barriers to sustained Petaflop Performance, invited talk at the 2006 Fall Creek Falls Conference, October 23-24, 2006.

Where Does MPI Need to Grow, invited presentation at Euro PVMMPI 2006, Bonn, Germany, September 18-20, 2006.

Three Questions You Should Ask, invited panel presentation at Clusters and Computational Grids for Scientific Computing, Asheville, NC, September 10-13, 2006.

Issues in Developing a Thread-Safe MPI Implementation, invited colloquia at the University of Utah, Salt Lake City, August 28, 2006.

Can There Be a Common Communication Runtime System?, High Productivity Computer Systems Languages Workshop, Oak Ridge, Tennessee, July 12-13, 2006.

Opportunities at Argonne National Laboratory, presented in the Workshop "Opportunities for Computing Research with Government Labs", CRA Conference at Snowbird 2006, Snowbird, Utah, June 25-27, 2006.

System Software Issues for the Future, invited panel presentation at the 2006 BG/L Consortium System Software and Applications workshop, Tokyo, Japan, April 19-20, 2006.

Overcoming the Barriers to Sustained Petaflop Performance, Invited presentation, Computational Science and Engineering Research Symposium (UIUC CSE day)

Thoughts on Capacity Computing, Invited panel presentation on Capacity Computing at SOS 10, March 6-8, 2006.

Beware of What You Wish For, Invited panel presentation on Data at SOS 10, Maui, Hawaii, March 6-8, 2006.

Some Thoughts on Programming Languages for HPC, Invited panel presentation at Architectures and Algorithms for Petascale Computing, Dagstuhl, Germany, February 12-17, 2006

Overcoming the Barriers to Sustained Petaflop Performance, Presentation at Architectures and Algorithms for Petascale Computing, Dagstuhl, Germany, February 12-17, 2006

A Science-Based Case for Large Scale Computation, Invited Keynote at SARA SuperDay, Amsterdam, The Netherlands, November 29, 2005.

How to Replace MPI as the Programming Model of the Future, Invited talk at Workshop on the Frontiers of Extreme Computing, Santa Cruz, CA, October 24-27, 2005.

Improving the Usability of Clusters, Invited Keynote at IEEE Cluster 2005, Boston, MA, September 26-29, 2005.

Towards a Productive MPI Environment, Invited talk at Euro PVMMPI, Sorento, Italy September 19-21, 2005.

Future Technologies that may Facilitate Science Breakthroughs Chair of Panel at SOS 9, Davos, Switzerland, March 21-23, 2005.

Some Myths in High Performance Computing, Invited dinner presentation at Northwest Indiana Computational Grid HPC Workshop, Purdue University, Indiana, March 8-9, 2005.

First Light with BlueGene/L At Argonne, Invited presentation at Northwest Indiana Computational Grid HPC Workshop, Purdue University, Indiana, March 8-9, 2005.

Is OpenMP for Users?, invited presentation at OpenMP BOF, Supercomputing 2004, Pittsburgh, November 7-12, 2004.

Grids and Clusters: Lessons for Deployment and Operation, Clusters and Computational Grids for Scientific Computing, Lyon, France, September 26-29, 2004.

MPI and High Productivity Programming, Invited talk at Euro PVMMPI, Budapest, Hungary, September 19-22, 2004.

Software for Exaflops Computing, Invited presentation at the Workshop on the Path to Extreme Supercomputing, LASCI 2004, October 12, Santa Fe, New Mexico.

How Not to Measure Performance: Lessons from Parallel Computing, presented at the Grid Performance Workshop 2004, London, UK, May 12-13, 2004.

The Triumph of Hope over Experience, invited panel presentation for visions of the future at SOS8, Charleston, SC, April 12-14, 2004.

MPICH2: A High-Performance, Portable Implementation of MPI, Invited presentation with Ewing Lusk at ClusterWorld Conference and Expo, April 5-8, 2004., San Jose, CA.

Algorithms and Architecture, invited presentation at the Advanced Computational Materials Science Workshop, Washington D.C., March 31-April 2, 2004.

Parallel Programming With MPI, invited guest lecture in APMA 4990 "Introduction to Parallel Scientific Computing", Columbia University, March 10, 2004.

Expressing Fault Tolerant Algorithms with MPI-2, at the Workshop on Fault Tolerance for MPI Implementors, SIAM Parallel Processing Meeting, San Francisco, CA, February 24, 2004.

Computer Algorithms and Architectures, invited presentation at Computation Institute Fellows Meeting, January, 2004.